

The Mixed Spin 3 - Spin 3/2 Ferrimagnetic Ising Model on Cellular Automaton

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The mixed spin 3- spin 3/2 Ising model has been simulated using standart and cooling algorithms on cellular automaton (CA). The simulations have been made in the interval $-6 \leq D \leq 6$ for $J = 1$ for the square lattices with periodic boundary conditions, including an anisotropy term D on spin-3. The model has compensation points through $D/J = 2$ line. The values of the critical exponents (ν , α , β and γ) are estimated within the framework of the finite-size scaling theory for selected D values (-2 , 0 , 1 , 2 and 4). The estimated values are compatible with the universal two dimensional Ising values.

I . INTRODUCTION

The mixed spin Ising model has been preferred as a simple model to study ferrimagnetism which plays the fundamental role in the area of molecular based magnetic materials. In the ferrimagnetic material, the existence of compensation point makes some technological applications possible such as the thermomag-

netic recording [1, 2]. The various mixtures of spins have been studied with the simulation and the numerical methods as effective field theory [3 – 5], Green’s function method [6], mean-field approximation [7 – 9], Buendia and Novotnys conjecture [10], density functional theory [11] and Monte Carlo [12 – 20]. However the mixed spin 3 - spin 3/2 Ising model has not been studied with any method yet. At the recent paper concerning the cyano-bridged terbium(*III*) - chromium(*III*) heterobimetallic assembly also attracted attention to absence of the study about spin 3- spin 3/2 mixture [21]. Therefore, the mixed spin 3- spin 3/2 Ising model is investigated via Cellular Automaton in this paper.

In the previous papers, the Creutz cellular automaton (CCA) algorithm and its improved versions have been used successfully to study the properties of the critical behaviors of the Ising model Hamiltonians [22 – 32] . The CCA algorithm, which was first introduced by Creutz [33] , is a microcanonical algorithm interpolating between the conventional Monte Carlo and the molecular dynamics techniques. Our previous studies showed that the cooling algorithm improved from the Creutz Cellular Automaton algorithm are effective to study the phase space and the critical behavior of the Ising model [34 – 39].

The aim of this study is to examine the critical behavior of the mixed spin 3- spin 3/2 Ising model. For this purpose, the order parameters (M , m_a , m_b ,

q_a, q_b), the susceptibility (χ), the internal energy (H_I) and the specific heat (C) were calculated on square lattice $L \times L$ of linear dimension $L = 32, 64, 128, 160$ and 256 with periodic boundary conditions. The $(kT_C/J, D)$ phase diagram in the interval $-6 \leq D \leq 6$ for $J = 1$ was obtained using the temperature value determined from the maxima of the susceptibility (χ) and the critical exponents were estimated by analyzing data within the framework of the finite-size scaling theory. The outline of this paper is as follows: In Section 2, the model and the formalism are given. In Section 3 the results and discussions are presented. In the final Section, a brief summary will be given.

II . Model

Two interpenetrating square sublattices occupied by the inequal spins composing the mixed-spin model. The Hamiltonian is given by

$$H_I = J \sum_{\langle ij \rangle} \sigma_i S_j + D \sum_i S_i^2 \quad (1)$$

where the sums are over all the nearest neighbors. J represents the bilinear interaction between spins $\sigma_i = \pm 3/2, \pm 1/2$ on sites of sublattice A and $S_i = \pm 3, \pm 2, \pm 1, 0$ on sites of sublattice B, D is a single ion anisotropy term on $S = 3$. The total energy H , which is conserved for the microcanonical algorithm, is given by

$$H = H_I + H_K \quad (2)$$

where H_I is Ising energy defined in equation (1) and H_K is kinetic energy. The kinetic energy H_K is an integer, equal to the change in the Ising spin energy for any spin flip. For a site belonging to sublattice A to be updated, its spin is changed to one of the other five states with $1/5$ probability. If a site belonging to sublattice B to be updated, its spin is changed to one of the other three states with $1/3$ probability. If this energy change is transferable to or from the kinetic energy variable of the site, considering the total energy H is conserved, then this change is done and kinetic energy is appropriately changed. Otherwise the spin is not change [34 – 37]. The simulations are carried out on the square lattice with $L = 32, 64, 128, 160$ and 256 for periodic boundary conditions.

At the cooling algorithm, the simulation consists of two parts, the initialization procedure and the computation of the thermodynamic quantities. In the initialization procedure, firstly, the sublattice A and B are decorated with S and σ , considering antiferromagnetic interaction ($J > 0$). The initial configuration for the cooling algorithm is obtained adding energy to the kinetic energy of 40% of the spins on the every sublattice for getting the disordered phase (P) at high temperature. The initial configuration is run during the 20.000 Cellular

Automaton time steps. During the cooling cycle, the kinetic energy (H_k) of 2% of the spins become equal to zero. Instead of resetting the starting configuration at each energy, it was used the final configuration at a given energy as the starting point for the next at cooling algorithm. The computed values of the thermodynamic quantities (the order parameter (M), sublattice order parameters (m_a , m_b), the susceptibility (χ , χ_a , χ_b), the Ising energy (H_I), the specific heat (C)) and the Binder cumulant (U_L) are averages over the lattice and over the number of time steps (2.000.000) with discard of the first 100.000 time steps during the cellular automaton develops [35].

Thermodynamic quantities are calculated by

$$m_a = \frac{2}{N} \sum_{i(even)} S_i, \quad m_b = \frac{2}{N} \sum_{i(odd)} \sigma_i \quad (3)$$

$$M = \frac{|m_a - m_b|}{2} \quad (4)$$

$$\chi = N \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT}, \quad \chi_a = \frac{N}{2} \frac{\langle m_a^2 \rangle - \langle m_a \rangle^2}{kT}, \quad \chi_b = \frac{N}{2} \frac{\langle m_b^2 \rangle - \langle m_b \rangle^2}{kT} \quad (5)$$

$$U_I = (J \sum_{\langle ij \rangle} S_i \sigma_j + D \sum_i S_i^2) / U_0 \quad (6)$$

$$C_I/k = N \frac{\langle U_I^2 \rangle - \langle U_I \rangle^2}{(kT)^2} \quad (7)$$

where U_0 is the ground state energy at $kT/J = 0$.

The phases are determined as

Paramagnetic (P): $m_a = m_b = 0$

Ferrimagnetic (f): $m_a \neq m_b \neq 0$

III. Results and Discussions

The ground state phase diagram in (D, J) is illustrated in figure 1 at the absolute zero temperature ($kT/J = 0$). It is seen that mixed spin 3- spin 3/2 Ising model has ferrimagnetic (f) and paramagnetic phase (P). Through $J = 1$, the mixed spin system has ferrimagnetic f_1 phase as the sublattice A and B occupied by $S = 3$ and $\sigma = -3/2$, respectively, in the interval $-6 \leq D < 1.2$. In the intervals $1.2 \leq D < 2$ and $2 < D \leq 5$, there are f_2 phase f_3 ferrimagnetic ground state phases, respectively. $S = 2$ and $\sigma = -3/2$ are located on the sublattice A and sublattice B creating ferrimagnetic f_2 while sublattices are decorated with $S = 1$ and $\sigma = -3/2$ in f_3 . Both f_3 and P phases appears in the interval $5 < D < 6$. For $D \leq 6$, there is paramagnetic phase (P). Through $D/J = 1.2$ phase separation line, $S = 3$ or 2 occupy the sublattice A while the sublattice B is decorated by $\sigma = -3/2$. Similarly, sublattice A is occupied

evenly by $S = 2$ or 1 while sublattice B is decorated by $\sigma = -3/2$ through $D/J = 2$ phase separation line. So the generated values of S are limited to smaller values with increasing D .

In figure 2, the temperature dependence of the sublattice order parameters are illustrated for selected $D = 1, 2$ and 4 values representing ferrimagnetic regions for $J = 1$. As it is seen in figure 2(a), the mixed spin system exhibits second order phase transition ($f \leftarrow P$). Both sublattice order parameters (m_a and m_b) appear continuous while the sublattice susceptibilities (χ_a and χ_b) have a characteristic peak at the same critical temperature for each D value. At $D = 2$, the sublattice order parameter m_a is equal to 1.5 while the sublattice order parameter m_b is equal to -1.5 cancelling each other for $0 \leq kT/J$, and hence there is a compensation point as Bobák et.al defined in the mixed spin-1 and spin-3/2 ferrimagnetic system [40]. The sublattice magnetizations (m_a and m_b) are illustrated for selected $J = 1, 2$ and 5 values through $D/J = 2$ line (figure 3). By this way it is verified that the sublattice order parameters (m_a and m_b) cancel each other for D values through the $D/J = 2$ line.

The lattice order parameters (M) and Ising energy (H_I) also appear continuous (figure 4(a) and (b)). The susceptibility (χ) and the specific heat (C) have a characteristic peak which shifts to higher temperatures with increasing D

value (figure 5(a) and (b)). It is obviously seen that single-ion anisotropy term D doesn't influence the phase transition type which is seen as of the second order. The simulations show that the mixed spin 3- spin 3/2 Ising system has second order phase transition from paramagnetic (P) phase to ferrimagnetic (f) phase ($f \leftarrow P$) using cooling algorithm in the interval $-6 \leq D \leq 6$. For $D \geq 6$, Ising energy doesn't exhibit any sign regarding a phase transition.

In figure 6, the phase diagram is shown on the $(kT_C/J, D)$ plane through $J = 1$ line estimating the critical temperatures from the susceptibility maxima. In the interval $-6 \leq D \leq 5$, the standart and the cooling algorithms give $P \rightarrow f$ second order phase transition at the same critical temperatures. However, standart algorithm still gives $f \rightarrow P$ second order phase transition for $5 < D < 6$, while there is no phase transition according to cooling algorithm results. The reason of this difference is occurrence of f_3 and P phases as ground states in the interval $5 < D < 6$. Thus, standart algorithm results initialized from the order state can exhibit f_3 ground state phase while cooling algorithm results show P phase as ground state.

The critical behavior of the quantities has been investigated within the framework of the finite size scaling theory for selected D values ($-2, 0, 1, 2$ and 4) through $J = 1$ line. In here, the figures are represented for $D = 1$ which

has f_1 ground state. The infinite lattice critical temperature $T_C(\infty)$ is obtained from the intersection point of the Binder cumulant curves for the different lattice sizes. As it is seen in figure 7(a), the Binder cumulant curves intersect at $T_C(\infty) = 4.61$. The critical exponent ν can be estimated using the finite-size scaling relation for the Binder cumulant given by

$$U_L = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2} \quad (8)$$

where reduced temperature is $\varepsilon = (T - T_C(\infty))/T_C(\infty)$. The scaling data for the Binder cumulant lie on a single curve for universal correlation critical exponent value $\nu = 1$ of two dimensional Ising model (figure 7(b)). $T_C(\infty)$ is also obtained by the finite-size scaling theory using following relation

$$T_C(\infty) = T_C(L) + aL^{-1/\nu} \quad (9)$$

Extrapolation of the susceptibility peak temperatures to $1/L^{1/\nu} \rightarrow 0$ gives us $T_C(\infty)$ value. Both from the intersection temperature value of the Binder cumulant curves and the extrapolation of the lattice susceptibility peak temperatures for different lattice sizes give $T_C(\infty) = 4.61$ at $D = 1$ (figure 7(c)).

In order to investigate the critical behaviors of the lattice order parameter (M), susceptibility (χ) and the specific heat (C), the following finite-size scaling

relations are used near the lattice critical temperature.

$$M = L^{-\beta/\nu} X(\varepsilon L^{1/\nu}) \quad (10)$$

$$kT\chi = L^{\gamma/\nu} Y(\varepsilon L^{1/\nu}) \quad (11)$$

$$C = L^{\alpha/\nu} Z(\varepsilon L^{1/\nu}) \quad (12)$$

The infinite lattice critical behaviors must be asymptotically reproduced for large $x = \varepsilon L^{1/\nu}$, that is,

$$X(x) = Bx^\beta \quad (13)$$

$$Y(x) = Cx^{-\gamma} \quad (14)$$

$$Z(x) = Ax^{-\alpha} \quad (15)$$

The finite-size scaling plots of the order parameter are exhibited in figure 8(a) at $D = 1$. For $\beta = 0.125$ and $\nu = 1$, data lie on a single curve both below $T_C(\infty)$ and above $T_C(\infty)$. For $T < T_C(\infty)$, the data of order parameter M are in good agreement with the universal value of $\beta = 0.125$. For $T > T_C(\infty)$, the

data fit to the straight line with $slope = \beta' = 0.875$ according to the equation (14). In figure 8(b), the finite size scaling plots of the data for the susceptibility are illustrated together the straight lines describing the theoretically predicted behavior for large x (equation (15)). The scaling of the susceptibility data agrees with the asymptotic form with $\gamma = \gamma' = 1.75$ and $\nu = 1$ for both sides of the $T_C(\infty)$. The specific heat of an infinite lattice is well described by

$$C/k = A\epsilon^{-\alpha} + b^{\pm} \quad (16)$$

where b^{\pm} expresses the nonsingular part of the specific heat [41]. The finite-size scaling plots of the singular portion of the specific heat $(C/k - b^{\pm})$ are shown in figure 8(c) and figure 8(d) for the selected $D = 1$ value. The data for the specific heat scale well with the values of $\alpha = 0.03$ at $T < T_C(\infty)$ and $\alpha' = 0.01$ at $T > T_C(\infty)$.

At $D = 2$ where m_a and m_b compensate, the infinite lattice critical temperature $T_C(\infty)$ is obtained as 2.96 ± 0.01 from the intersection point of the Binder cumulant curves (figure 9(a)) and from the extrapolation of the susceptibility peak temperatures to $1/L^{1/\nu} \rightarrow 0$ (figure 9(c)) for the different lattice sizes. On the other hand the universal correlation critical exponent value is obtained as $\nu = 1$ from the scaling of the Binder cumulant (figure 9(b)). In figure 10, the

critical exponents are estimated for $D = 2$ where the m_a and m_b cancel each other. They are estimated as $\nu = 1$, $\beta = 0.125$, $\beta' = 0.875$, $\gamma = \gamma' = 1.75$, $\alpha = 0.05$ and $\alpha' = 0.04$ within the framework of the finite-size scaling theory are compatible with theoretical values.

The estimated values of the critical exponents (α , α' , β , β' , γ , γ' and ν), the infinite critical temperatures as well as b^\pm are given in table 1 for selected D values ($-2, 0, 1, 2$ and 4) through $J = 1$ line. As it is seen from table 1 that, the estimated critical exponents are in good agreement with theoretical ones ($\nu = 1$, $\alpha = \alpha' = 0$, $\beta = 0.125$, $\beta' = 0.875$ and $\gamma = \gamma' = 1.75$).

Table 1. The estimated values of the critical exponents					
	D = -2	D = 0	D = 1	D = 2	D = 4
$T_C^{UL}(\infty)$	7.46 ± 0.01	5.99 ± 0.01	4.61 ± 0.01	2.96 ± 0.01	1.46 ± 0.01
$T_C^X(\infty)$	7.46 ± 0.01	5.99 ± 0.01	4.61 ± 0.01	2.97 ± 0.01	1.46 ± 0.01
b^-	-0.01	-0.06	-0.01	-0.015	-0.05
b^+	-0.02	-0.07	-0.03	-0.050	0.00
ν	1	1	1	1	1
α	0.010	0.008	0.030	0.050	0.030
α'	0.010	0.020	0.010	0.040	0.050
β	0.125	0.125	0.125	0.125	0.125
β'	0.875	0.875	0.875	0.875	0.875
γ	1.75	1.75	1.75	1.75	1.75
γ'	1.75	1.75	1.75	1.75	1.75

III. SUMMARY

The two dimensional spin 3- spin 3/2 mixed spin Ising model has been simulated using cooling algorithm on the cellular automaton (CA) for the square lattices in the interval $-6 \leq D \leq 6$. The simulations show that the spin system with antiferromagnetic interaction has ferrimagnetic (f_1 , f_2 , f_3) and param-

agnetic (P) phases at absolute zero temperature ($kT/J = 0$). The existence of single-ion anisotropy term D does not effect the phase transition type but the phase transition temperatures shift to the low temperatures with its increasing value. As it is recognized from the (D, J) phase diagram that the generated values of S are limited to smaller values with increasing values of D . An other result is occurrence of the compensation points through $D/J = 2$ line at $kT/J = 0$. For selected D values ($-2, 0, 1, 2$ and 4) through $J = 1$ line, the estimated values of the critical exponents which are independent from D value are in a good agreement with universal values of the two dimensional Ising model. The standart and the cooling algorithm are suitable procedures for simulating mixed spin systems.

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Figure Captions

Figure 1. The ground state phase diagram of the mixed Spin 3–spin 3/2

ferrimagnetic Ising model. f and P indicate ferrimagnetic and paramagnetic phases, respectively. On the phase separation line between ferrimagnetic f_1 and f_2 phases there is ferrimagnetic f_3 phase.

Figure 2. The temperature dependence of the (a) sublattice magnetizations (m_a, m_b) and (b) the susceptibilities (χ_a, χ_b).

Figure 3. The temperature dependence of the sublattice order parameters (m_a and m_b) through $D/J = 2$ line for $J = 1, 2$ and 5 .

Figure 4. Temperature dependences of (a) Lattice order parameter (M) and (b) Ising energy (H_I) .

Figure 5. Temperature dependences of (a) lattice susceptibility (χ) and (b) The specific heat (C/k) .

Figure 6. Phase diagram of the mixed spin 3- spin 3/2 Ising model on ($kT_C/J, D$) plane for $J = 1$. Thick line and square symbol indicate the standart and the cooling algorithm results, respectively. Vertical thin lines are used for separating ground state regions.

Figure 7. For $D = 1$ and $J = 1$; (a) Temperature estimations from the intersection point of the Binder curves, (b) The estimation for the critical exponent ν from Binder cumulant scaling and (c) Temperature estimations from the linear extrapolation.

Figure 8. For $D = 1$ and $J = 1$; finite-size scaling plots of (a) the lattice order parameter (M), (b) the susceptibility (χ), (c) the specific heat (C) at $T < T_C$ and (d) the specific heat (C) $T > T_C$.

Figure 9. For $D = 2$ and $J = 1$; (a) Temperature estimations from the intersection point of the Binder curves, (b) The estimation for the critical exponent ν from Binder cumulant scaling and (c) Temperature estimations from the linear extrapolation.

Figure 10. For $D = 2$ and $J = 1$; finite-size scaling plots of (a) the lattice order parameter (M), (b) the susceptibility (χ), (c) the specific heat (C) at $T < T_C$ and (d) the specific heat (C) $T > T_C$.



















